

# LATTICE COLOR GROUPS OF QUASICRYSTALS

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Lattice color groups are introduced and used to study the partitioning of a periodically- or quasiperiodically-ordered set of points into  $n$  symmetry-related subsets. Applications range from magnetic structure to superlattice ordering in periodic and quasiperiodic crystals.

## 1 Introduction

It is well known that the points of a square lattice may be partitioned into two square subsets, related by a translation, but that the same is not true for triangular lattices. This allows a certain kind of anti-ferromagnetic order in tetragonal crystals which is not possible for hexagonal crystals. One often encounters similar situations in which a set of lattice points is to be partitioned into  $n$  “symmetry-related” subsets (to be properly defined below). If the lattice points correspond, for example, to atomic positions in a crystal then the different subsets may correspond to different chemical species or to  $n$  different orientations of a magnetic moment. One may also single out just one of the subsets to play a significant role such as in describing superlattice ordering. We shall address here the generalization of this question to quasiperiodic crystals. In doing so we shall introduce some aspects of the theory of color symmetry for periodic and quasiperiodic crystals.<sup>1</sup> Please consult Ref. 1 for complete detail and a rigorous derivation of the results given here.

## 2 Color symmetry

By associating one of  $n$  distinct colors with each site of a crystal one produces a *colored crystal* and a partitioning, as described above. The colored crystal is said to have *color symmetry* if rotations (and, in the special case of periodic crystals, translations) that are symmetry operations of the uncolored crystal may be combined with global permutations of the  $n$  colors to become symmetry operations of the colored crystal.

What do we mean when we say that a rotation is a symmetry of a quasiperiodic crystal? In the case of periodic crystals we mean that the rotation leaves the crystal *invariant* to within a translation, but this is in general not the case for quasicrystals. The key to redefining symmetry for quasiperiodic crystals is the notion of indistinguishability. Two crystals are *indistinguishable* if

Table 1: Indices of invariant sublattices of standard 2-dimensional  $N$ -fold lattices, giving the possible numbers of colors in a symmetric partitioning of a 2-dimensional  $N$ -fold quasicrystal. The sublattices are only required to be invariant under the point group  $G = n$  and not under the full point group of the  $N$ -fold lattice which also contains mirror reflections.

Lattice order $N$	Point Group $G$	Indices of sublattices, invariant under $G = n$
Rank 2		
4	4	1, 2, 4, 5, 8, 9, 10, 13, 16, 17, 18, 20, 25, 26, 29, 32, 34, 36, 37, ...
6	3, 6	1, 3, 4, 7, 9, 12, 13, 16, 19, 21, 25, 27, 28, 31, 36, 37, 39, 43, ...
Rank 4		
8	8	1, 2, 4, 8, 9, 16, 17, 18, 25, 32, 34, 36, 41, 49, 50, 64, 68, 72, ...
10	5, 10	1, 5, 11, 16, 25, 31, 41, 55, 61, 71, 80, 81, 101, 121, 125, 131, ...
12	12	1, 4, 9, 13, 16, 25, 36, 37, 49, 52, 61, 64, 73, 81, 97, 100, 109, ...
Rank 6		
14	7, 14	1, 7, 8, 29, 43, 49, 56, 64, 71, 113, 127, 169, 197, 203, 211, 232, ...
18	9, 18	1, 3, 9, 19, 27, 37, 57, 64, 73, 81, 109, 111, 127, 163, 171, 181, ...
Rank 8		
16	16	1, 2, 4, 8, 16, 17, 32, 34, 49, 64, 68, 81, 97, 113, 128, 136, 162, ...
20	20	1, 5, 16, 25, 41, 61, 80, 81, 101, 121, 125, 181, 205, 241, 256, ...
24	24	1, 4, 9, 16, 25, 36, 49, 64, 73, 81, 97, 100, 121, 144, 169, 193, ...
30	15, 30	1, 16, 25, 31, 61, 81, 121, 151, 181, 211, 241, 256, 271, 331, ...

they contain the same spatial distribution of bounded substructures of arbitrary size. For a (proper or improper) rotation to be in the *point group*  $G$  of a quasiperiodic crystal it is only required to leave it indistinguishable and not necessarily invariant. It can be shown that if two *periodic* crystals are indistinguishable then they differ at most by a translation, thus reducing the new definition of point group back to the traditional one. A more detailed account of these concepts and their use in generalizing crystallography to treat quasiperiodic crystals may be found elsewhere.<sup>2</sup>

The point group  $G$  of a colored quasiperiodic crystal is subsequently defined as the set of rotations which leave it indistinguishable to within a permutation of the colors. The *color point group* of the crystal consists of all pairs  $(g, \gamma)$  leaving it indistinguishable, where the  $g$ 's are elements of the point group  $G$  and the  $\gamma$ 's are color permutations. In general, there can be many different  $\gamma$ 's associated with a single point group rotation  $g$ . Of particular interest are the color permutations which may be paired with the identity rotation to leave the colored crystal indistinguishable. These color permutations form the *lattice color group* which is the focus of our discussion here. In the special case of periodic crystals these are permutations which when combined with a translation leave the crystal invariant.

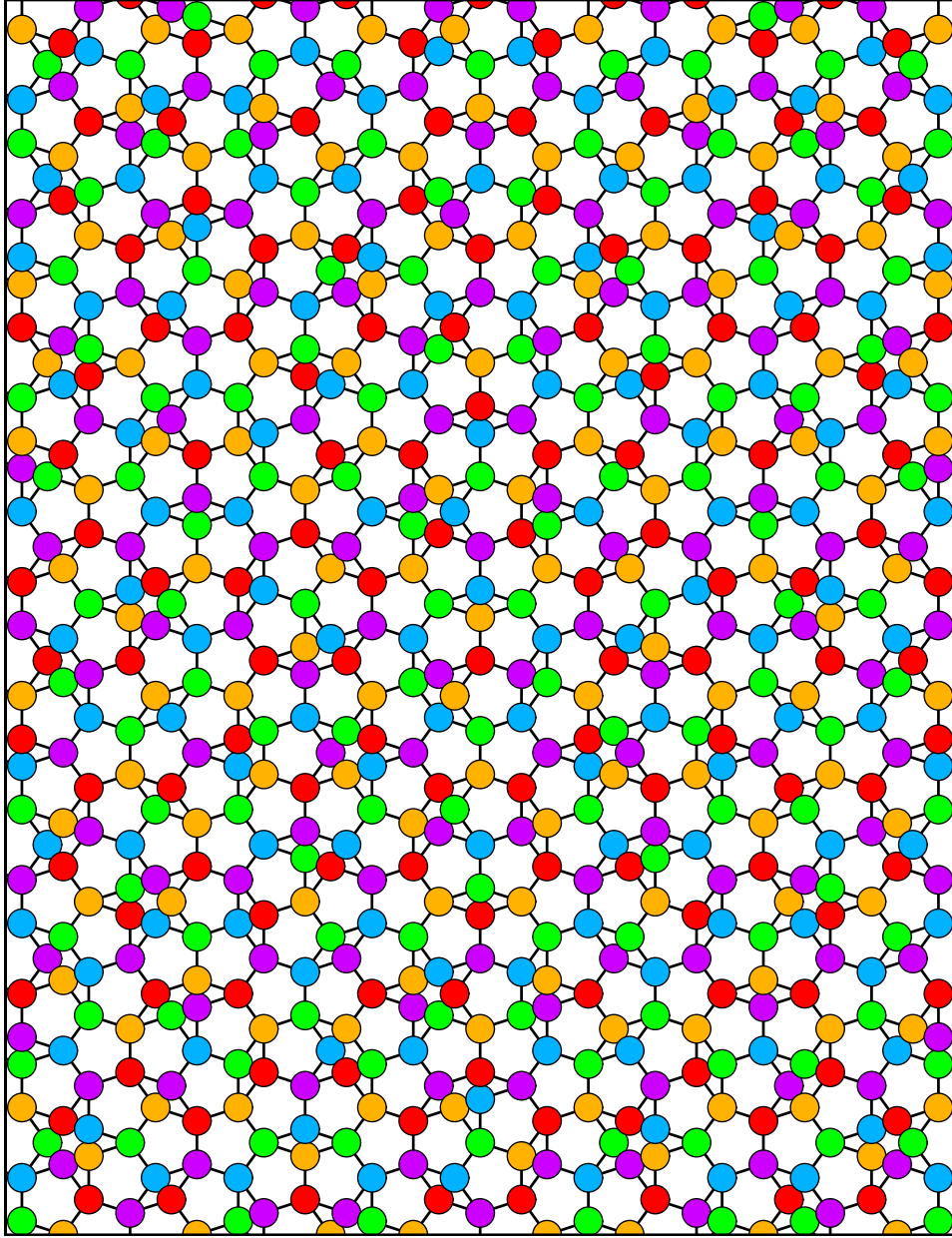


Figure 1: A symmetric partitioning with 5 colors of the vertices of a 10-fold Penrose tiling, originally introduced by Lück.<sup>7</sup> The lattice color group is the cyclic group of order 5, generated by the permutation (red, purple, blue, green, orange).

### 3 Lattice Color Groups and Invariant Sublattices

For the purpose of our discussion here we define a *symmetric partitioning* of a quasiperiodically-ordered set of points to be an  $n$ -coloring of the set, satisfying the following requirements: (a) The point group  $G$  of the colored set is the same as that of the uncolored one; and (b) the lattice color group is transitive on the  $n$  colors. To elaborate, we require that any rotation in the point group of the uncolored set of points may be combined with a color permutation to leave the colored set indistinguishable, and that for any pair of differently-colored subsets there exists at least one permutation in the lattice color group, taking one into the other. It follows from (a) and (b) that each individually-colored subset is also left indistinguishable by the elements of  $G$ .

Colored periodic crystals, satisfying the requirements above, have been studied previously.<sup>3</sup> To each element of the crystal's periodic lattice  $T$  of translations corresponds a unique color permutation. One finds that the sublattice  $T_0$ , associated with the identity color permutation, is invariant under the point group  $G$  of the crystal; its index in  $T$  is equal to the number of colors  $n$ ; and the quotient group  $T/T_0$  is isomorphic to the lattice color group. The classification of lattice color groups, compatible with crystals with a given lattice  $T$  and point group  $G$ , thus reduces to the classification of sublattices  $T_0$  of  $T$  that are invariant under  $G$ .

In the case of quasiperiodic crystals one has no lattice of translations but as it turns out,<sup>1</sup> a similar situation arises in Fourier space which holds both for periodic and quasiperiodic crystals. The (Fourier) lattice  $L_0$  (called by some “the Fourier module”), consisting of all the wave vectors appearing in the diffraction diagram of the uncolored crystal, is a sublattice of the (Fourier) lattice  $L$ , consisting of all the wave vectors that would appear in a diffraction diagram due to the sites of a single color in the colored crystal. This is a phenomenon, familiar from structures with superlattice ordering, where additional weak satellites appear in the diffraction diagram turning the original lattice  $L_0$  into  $L$ . Such diffraction diagrams, exhibiting superstructure ordering, have been observed in decagonal AlCoNi quasicrystals<sup>4</sup> as well as in icosahedral AlPdMn quasicrystals.<sup>5</sup>

One finds that the sublattice  $L_0$  is invariant under the point group  $G$  of the full lattice  $L$ ; the index of  $L_0$  in  $L$  is equal to the number of colors; and the quotient group  $L/L_0$  is isomorphic to the lattice color group. Again, the classification of lattice color groups is reduced to the classification of invariant (Fourier) sublattices.

Consider as a first example the partitioning of a standard 2-dimensional  $N$ -fold quasicrystal ( $N < 46$ ) into *two* indistinguishable parts, allowing the

type of anti-ferromagnetic order discussed in the introduction. The lattice  $L$  of a standard  $N$ -fold quasicrystal may be generated by an  $N$ -fold star of wave vectors of equal length. For the required partitioning,  $L$  must contain an invariant sublattice  $L_0$  of index 2. One can show that any sum, containing an *odd* number of vectors from the generating star, must not belong to  $L_0$ . It then follows that invariant sublattices of index 2 can exist only if  $N$  is a power of 2. Niizeki<sup>6</sup> has shown such a 2-coloring of the vertices of an octagonal tiling.

Consider finally the possible values of  $n$ , compatible with a symmetric partitioning of a given standard 2-dimensional  $N$ -fold quasicrystal ( $N < 46$ ). Because all  $N$ -fold lattices with  $N < 46$  are standard any invariant sublattice must itself be a standard  $N$ -fold lattice. Any arbitrary vector  $\mathbf{k} \in L$  belongs to an  $N$ -fold star which generates a sublattice  $L_0$  of  $L$ . One can thus generate all the sublattices of  $L$  simply by letting  $\mathbf{k}$  run through all wave vectors in  $L$ . The index of the sublattice is just the magnitude of the determinant of the matrix which gives the basis of  $L_0$  in terms of the basis of  $L$ . Results for lattices up to rank 8, taken from Ref. 1, are reproduced in Table 1. An example of a 5-coloring of the vertices of a decagonal Penrose tiling, first introduced by Lück,<sup>7</sup> is shown in Figure 1. A different approach for calculating invariant sublattices, which involves generating functions of Dirichlet series, is used by Baake *et al.*<sup>8</sup> and yields the same results.

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